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On the Phase Transition Phenomenon of Graph Laplacian Eigenfunctions on Trees

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Abstract

We discuss our current understanding on the phase transition phenomenon of the graph Laplacian eigenfunctions constructed on a certain type of trees, which we previously observed through our numerical experiments. The eigenvalue distribution for such a tree is a smooth bell-shaped curve starting from the eigenvalue 0 up to 4. Then, at the eigenvalue 4, there is a sudden jump. Interestingly, the eigenfunctions corresponding to the eigenvalues below 4 are *semi-global* oscillations (like Fourier modes) over the entire tree or one of the branches; on the other hand, those corresponding to the eigenvalues above 4 are much more *localized* and *concentrated* (like wavelets) around junctions/branching vertices. For a special class of trees called *starlike trees*, we can now explain such phase transition phenomenon precisely. For a more complicated class of trees representing neuronal dendrites, we have a conjecture based on the numerical evidence that the number of the eigenvalues larger than 4 is bounded from above by the number of vertices whose degrees is strictly larger than 2. We have also identified a special class of trees that are the only class of trees that can have the exact eigenvalue 4.

1 Introduction

More and more data are collected in a distributed and irregular manner due to the advent of sensor technology. Such data are not so organized as familiar digital signals and images sampled on regular lattices. Examples include data measured on sensor networks, social networks, webpages, biological networks, and so on. Such unorganized data can be conveniently represented as a graph where each vertex represents a sensor or measured data by a sensor and each edge represents a relationship (e.g., a physical or wireless connectivity or a certain measure of affinity, etc.) between two vertices connected by that edge. Moreover, constructing a graph from a usual signal or image and analyzing it can also lead to a very powerful tool (e.g., the nonlocal mean denoising algorithm of Buades, Coll, and Morel [1]). Hence, it is very important to transfer harmonic and wavelet analysis techniques, which were originally developed on the usual Euclidean spaces and proven to be useful for so many practical problems associated with usual signals and images, to graphs and networks. Examples of such effort includes spectral graph wavelet transform of Hammond, Vandergheynst, and Gribonval [8] and the tensor-product Haar-like basis for digital databases proposed by Coifman, Gavish, and Nadler [3, 5], to name just a few. As sines, cosines, and complex exponentials play a fundamental role in harmonic analysis on the Euclidean spaces, the graph Laplacian eigenfunctions play such a role on graphs (note that the sines, cosines, and complex exponentials are the Laplacian eigenfunctions for an interval with the Dirichlet, Neumann, and periodic boundary conditions, respectively). Hence, it is of crucial importance to understand the behavior of the graph Laplacian eigenfunctions of a given graph. In this short note, we will describe our effort to understand the surprising behavior of the graph Laplacian eigenfunctions on trees that we discovered previously [9]: some of them are global oscillations like Fourier modes and the others are localized wiggles like wavelets depending on the corresponding eigenvalues.

In our previous report [9], we proposed a method to characterize dendrites of neurons, more specifically retinal ganglion cells (RGCs) of a mouse, and cluster them into different cell types using their morphological features, which are derived from the eigenvalues of the graph Laplacians when such dendrites are represented as graphs (in fact literally as "trees"). For the details on the data acquisition and the conversion of dendrites to graphs, see [9] and references therein. While analyzing the eigenvalues and eigenfunctions of those graph Laplacians, we observed a very peculiar *phase transition phenomenon* as shown in Figure 1. In other words, the eigenvalue distribution for each dendritic tree is a smooth bell-shaped curve starting from the eigenvalue 0 up to 4. Then, at the eigenvalue 4, there is a sudden jump as shown in Figure 1(c, d). Interestingly, the eigenfunctions corresponding to the eigenvalues below 4 are *semi-global* oscillations (like Fourier cosines/sines) over the entire dendrites or one of the dendrite arbors (or branches); on the other hand, those corresponding to the eigenvalues above 4 are much more *localized* and *concentrated* (like wavelets) around junctions/branching vertices, as shown in Figure 2.

We want to answer the following questions:

Q1 Why does such a phase transition phenomenon occur?

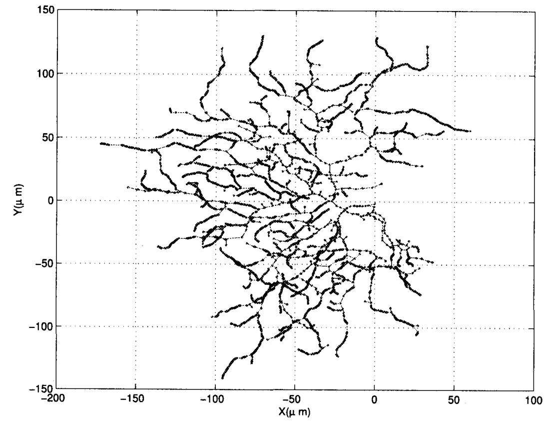
Q2 What is the significance of the eigenvalue 4?

Q3 Is there any tree that possesses the exact eigenvalue 4?

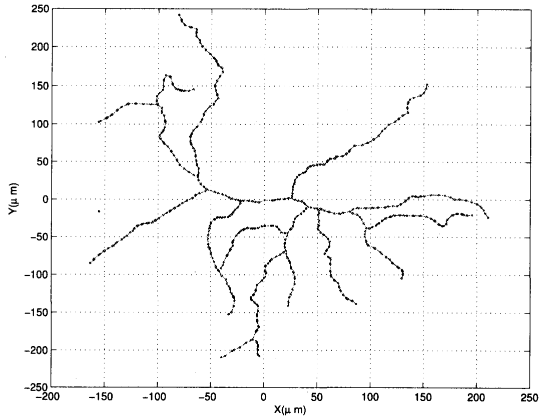
At this point of time, we have a complete answer to Q3, which will be described in Section 5. As for Q1 and Q2, we have a complete answer for a specific and simple class of trees called *starlike trees* as described in Section 3, and a partial answer for more general trees such as those representing neuronal dendrites, which we will discuss in Sections 4 and 6.

2 Definitions and Notation

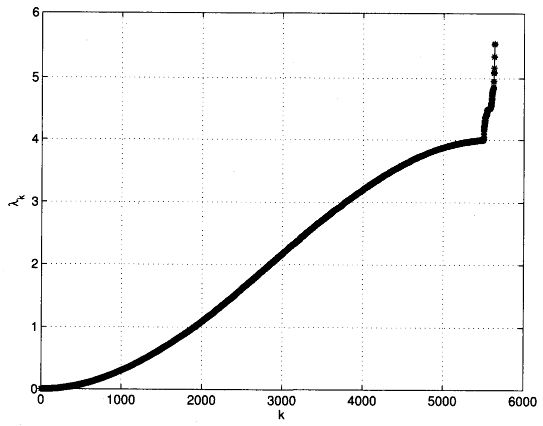
Let G be a graph representing dendrites of an RGC, and let $V(G) = \{v_1, v_2, \ldots, v_n\}$ be a set of vertices in G where each $v_k \in \mathbb{R}^3$ represents a sampled point (in the 3D coordinate system) along dendritic arbors of this RGC. Let $E(G) = \{e_1, e_2, \ldots, e_m\}$ be a set of edges where e_k connects two vertices v_i, v_j for some $1 \le i, j \le n$, and we write $e_k = (v_i, v_j)$. Let $d(v_k) = d_{v_k}$ be the degree of the vertex v_k. In fact, dendrites of each RGC in our dataset



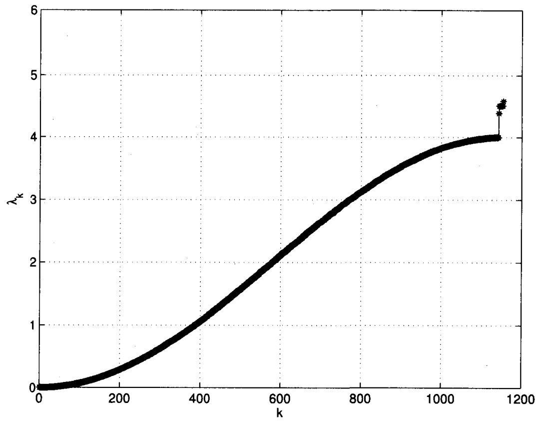
(a) RGC #60



(b) RGC #100

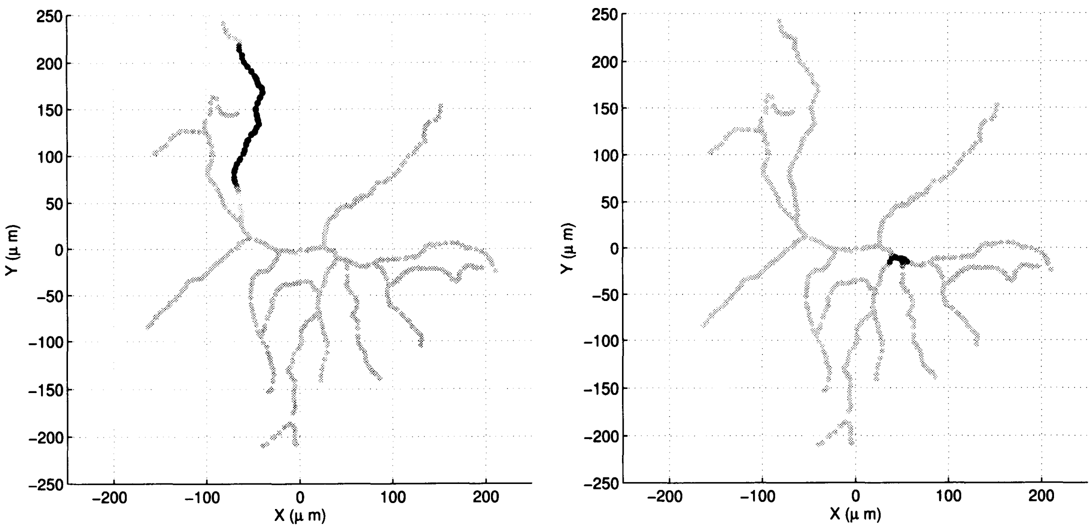


(c) Eigenvalues of (a)



(d) Eigenvalues of (b)

Figure 1: Typical dendrites of Retinal Ganglion Cells (RGC) of a mouse and the graph Laplacian eigenvalue distributions. (a) 2D projection of dendrites of RGC of a mouse; (b) that of another RGC revealing different morphology; (c) the eigenvalue distribution of RGC shown in (a); (d) that of RGC shown in (b). Regardless of their morphological features, a phase transition occurs at the eigenvalue 4.



(a) RGC #100; $\lambda_{1141} = 3.9994$ (b) RGC #100; $\lambda_{1142} = 4.3829$

Figure 2: The graph Laplacian eigenfunctions of RGC #100. (a) The one corresponding to the eigenvalue $\lambda_{1141} = 3.9994$, immediately below the value 4; (b) the one corresponding to the eigenvalue $\lambda_{1142} = 4.3829$, immediately above the value 4.

can be converted to a *tree* rather than a general graph since it is connected and contains no cycles; see [9] for the details. We also note that we only deal with *un*weighted graphs in this paper. In other words, we essentially examine the connectivities, topology, and complexity of the dendritic trees, which may not reflect the physical lengths and widths of the dendritic arbors; we are currently investigating weighted graphs where the weights are related to the physical distances between vertices, and hope that we can report our findings at a later date. Let $L(G) := D(G) - A(G)$ be the *(combinatorial) Laplacian matrix* where $D(G) := \mathrm{diag}(d_{v_1}, \ldots, d_{v_n})$ is called the *degree matrix* of G, i.e., the diagonal matrix of vertex degrees, and $A(G) = (a_{ij})$ is the *adjacency matrix* of G, i.e., $a_{ij} = 1$ if v_i and v_j are adjacent; otherwise it is 0. Furthermore, let $0 = \lambda_0(G) \le \lambda_1(G) \le \cdots \le \lambda_{n-1}(G)$ be the sorted eigenvalues of $L(G)$. Let $m_G(\lambda)$ be the multiplicity of the eigenvalue λ. More generally, if $I \subset \mathbb{R}$ is an interval of the real line, then we define $m_G(I) := \#\{\lambda_k(G) \in I\}$.

At this point we would like to give a simple yet important example of a tree and its graph Laplacian: a *path* graph consisting of n vertices shown in Figure 3. The graph

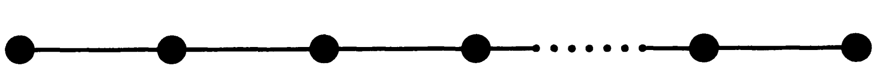


Figure 3: A path graph provides a simple yet important example.

Laplacian of such a path graph can be easily obtained and is instructive.

$$L(G) = D(G) - A(G)$$

$$\begin{bmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & & & & & \\ & 2 & & & & \\ & & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & \\ & & & & & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & & & & \\ 1 & 0 & 1 & & & \\ & 1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & 0 & 1 \\ & & & & 1 & 0 \end{bmatrix}.$$

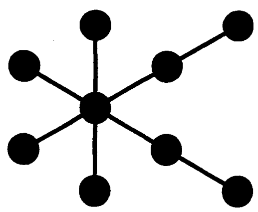
The eigenvectors[1] of this matrix are nothing but the *DCT Type II* basis vectors used for the JPEG image compression standard; see e.g., [10]. In fact, we have

- $\lambda_k = 2 - 2\cos(\pi k/n) = 4\sin^2(\pi k/2n),\ k = 0, 1, \ldots, n-1;$
- $\boldsymbol{\phi}_k = \left(\cos(\pi k(j+\frac{1}{2})/n)\right)^{\mathrm{T}}_{0 \le j < n},\ k = 0, 1, \ldots, n-1.$

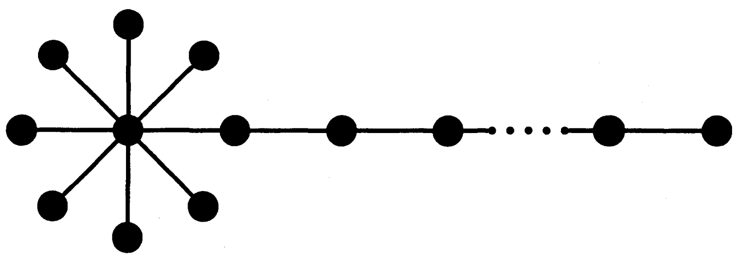
Note that for any finite $n \in \mathbb{N}$, $\lambda_{\max} = \lambda_{n-1} \lneqq 4$, and no localization/concentration occurs in the eigenvector $\boldsymbol{\phi}_{n-1}$, which is simply a global oscillation with the highest possible (i.e., the Nyquist) frequency, i.e., $\boldsymbol{\phi}_{n-1} = \left((-1)^j \sin(\pi(j+\frac{1}{2})/n)\right)^{\mathrm{T}}_{0 \le j < n}$.

3 Analysis of Starlike Trees

As one can imagine, analyzing this phase transition phenomenon for complicated dendritic trees turns out to be rather difficult. Hence, we start our analysis on a simpler class of trees called *starlike trees*. A starlike tree is a tree that has exactly one vertex of degree greater than 2. Examples are shown in Figure 4. We use the following notation. Let



(a) $S(2,2,1,1,1,1)$



(b) $S(n_1,1,1,1,1,1,1,1)$ a.k.a. comet

Figure 4: Typical examples of a starlike tree.

$S(n_1, n_2, \ldots, n_k)$ be a starlike tree that has $k(\ge 3)$ paths (i.e., branches) emanating from the central vertex v_1. Let the ith branch have n_i vertices excluding v_1. Let $n_1 \ge n_2 \ge \cdots \ge n_k$. Hence, the total number of vertices is $n = 1 + \sum_{i=1}^{k} n_i$.

[1] In this paper, we use the terms eigenvectors and eigenfunctions interchangeably.

Soon after we proved in 2010 the largest eigenvalue for a comet (a special class of starlike trees as shown in Figure 4 (b)) is always larger than 4, we noticed the following more general results for any starlike tree obtained by Das in 2007 [4]:

$$\lambda_{\max} = \lambda_{n-1} < k + 1 + \frac{1}{k-1}; \tag{1}$$

$$2 + 2\cos\left(\frac{2\pi}{2n_k+1}\right) \le \lambda_{n-2} \le 2 + 2\cos\left(\frac{2\pi}{2n_1+1}\right). \tag{2}$$

On the other hand, Grone and Merris [6] proved the following lower bound for a general graph G with at least one edge:

$$\lambda_{\max} \ge \max_{1\le j\le n} d(v_j) + 1. \tag{3}$$

Hence we have the following

Corollary 3.1. *A starlike tree has exactly one graph Laplacian eigenvalue greater than or equal to* 4. *The equality holds if and only if the starlike tree is* $K_{1,3} = S(1,1,1)$, *which is also known as a* claw.

Proof. The first statement is easy to show. The lower bound in (3) is larger than or equal to 4 for any starlike tree since $\max_{1\le j\le n} d(v_j) = d(v_1) \ge 3$. On the other hand, the second largest eigenvalue λ_{n-2} clearly cannot exceed 4 due to (2). The second statement about the necessary and sufficient condition on the equality requires the argument in Section 5, in particular, Corollary 5.2. From this, we can easily see that the only starlike tree having the exact eigenvalue 4 is $K_{1,3}$. □

As for the concentration/localization of the eigenfunction $\boldsymbol{\phi}_{n-1}$ corresponding to the largest eigenvalue λ_{n-1}, very recently we have proved the following

Theorem 3.2. *Let* $\boldsymbol{\phi}_{n-1} = \left(\phi_{1,n-1}, \cdots, \phi_{n,n-1}\right)^{\mathrm{T}}$, *where* $\phi_{j,n-1}$ *is the value of the eigenfunction corresponding to the largest eigenvalue* λ_{n-1} *at the vertex* v_j, $j = 1, \ldots, n$. *Then, the absolute value of this eigenfunction at the central vertex* v_1 *cannot be exceeded by those at the other vertices, i.e.,*

$$|\phi_{1,n-1}| > |\phi_{j,n-1}|, \quad j = 2, \ldots, n.$$

The details of the proof will appear elsewhere. We note that Das proved this theorem for a homogeneous starlike tree, $S(m, m, \cdots, m)$ in [4], and our theorem is for a general starlike tree.

Remark 3.3. Let $\boldsymbol{\phi} = (\phi_1, \phi_2, \ldots, \phi_n)^{\mathrm{T}}$ be an eigenvector of a starlike tree $S(n_1, \ldots, n_k)$ corresponding to the eigenvalue λ. Let $v_2, \ldots, v_{n_1+1}$ be the n_1 vertices along a branch emanating from the central vertex v_1 with v_{n_1+1} being the leaf vertex. Then, along this branch, the eigenvector components satisfy the following equations:

$$\begin{aligned} \lambda\phi_{n_1+1} &= \phi_{n_1+1} - \phi_{n_1} && (4)\\ \lambda\phi_j &= 2\phi_j - \phi_{j-1} - \phi_{j+1} \quad 2 \le j \le n_1. && (5) \end{aligned}$$

From Eq. (5), we have the following recursion relation:

$$\phi_{j+1} + (\lambda - 2)\phi_j + \phi_{j-1} = 0, \quad j = 2, \ldots, n_1. \tag{6}$$

This recursion can be explicitly solved using the roots of the characteristic equation

$$r^2 + (\lambda - 2)r + 1 = 0, \tag{7}$$

and the general solution can be written as

$$\phi_j = A r_1^{j-2} + B r_2^{j-2}, \quad j = 2, \ldots, n_1 + 1, \tag{8}$$

where r_1, r_2 are the roots of (7), and A, B are appropriate constants derived from the boundary condition (4). Now, let us consider these roots of (7) in details. The determinant of (7) is

$$\mathcal{D}(\lambda) := (\lambda - 2)^2 - 4 = \lambda(\lambda - 4). \tag{9}$$

Since we know that $\lambda \geq 0$, this determinant changes its sign depending on $\lambda < 4$ or $\lambda > 4$. (Note that $\lambda = 4$ occurs only for the claw $K_{1,3}$ on which we explicitly know everything; hence we will not discuss this case further in this remark.) If $\lambda < 4$, then $\mathcal{D}(\lambda) < 0$ and it is easy to show that the roots are complex valued with magnitude 1. This implies that (6) becomes

$$\phi_j = A' \cos(\omega(j-2)) + B' \sin(\omega(j-2)), \quad j = 2, \ldots, n_1 + 1, \tag{10}$$

where ω satisfies $\tan\omega = \sqrt{\lambda(4-\lambda)}/(2-\lambda)$, and A', B' are appropriate constants. In other words, if $\lambda < 4$, the eigenfunction along this branch is of oscillatory nature. On the other hand, if $\lambda > 4$, then $\mathcal{D}(\lambda) > 0$ and it is easy to show that both r_1 and r_2 are real valued with $-1 < r_1 = \left(2 - \lambda + \sqrt{\lambda(\lambda-4)}\right)/2 < 0$ while $r_2 = \left(2 - \lambda - \sqrt{\lambda(\lambda-4)}\right)/2 < -1$. It is clear that the dominating part is the term $B r_2^{j-2}$ in (8). The siuation is the same for the other branches. This observation has lead us to the proof of Theorem 3.2, which we defer to our forthcoming paper. In summary, for a starlike tree, the phase transition phenomenon with the eigenvalue 4 is hence essentially explained and well understood.

4 Our Conjecture

Unfortunately, actual dendritic trees are not exactly starlike. However, our numerical computations and data analysis indicate that:

$$0 \leq \frac{\#\{j \in (1,n) \mid d(v_j) \gneqq 2\} - m_G([4,\infty))}{n} \leq 0.047 \tag{11}$$

for each RGC we examined. Hence, we can define *starlikeliness* $S\ell(T)$ of a given tree T as

$$S\ell(T) := 1 - \frac{\#\{j \in (1,n) \mid d(v_j) \gneqq 2\} - m_T([4,\infty))}{n} \tag{12}$$

We note that $S\ell(T) \equiv 1$ for a certain class of RGCs whose dendrites are widely and sparsely spread (see [9] for the characterization). This means that dendrites in that class are all close to a starlike tree or a concatenation of several starlike trees. We show some examples of dendritic trees with $S\ell(T) \equiv 1$ and those with $S\ell(T) \lneqq 1$ in Figures 5, 6, and 7.

Based on our intensive numerical experiments, we have the following

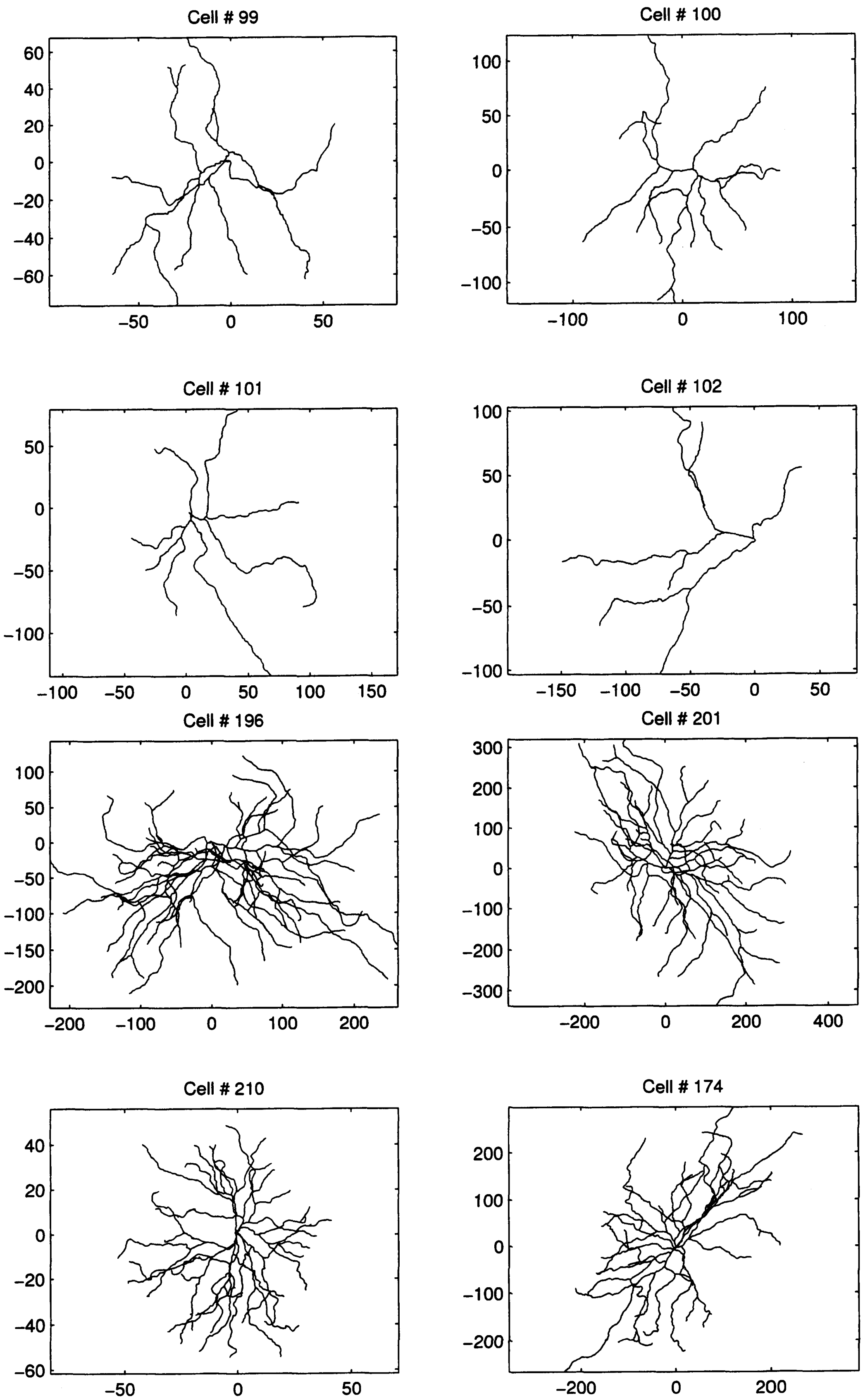


Figure 5: Examples of dendritic trees with $S\ell(T) \equiv 1$.

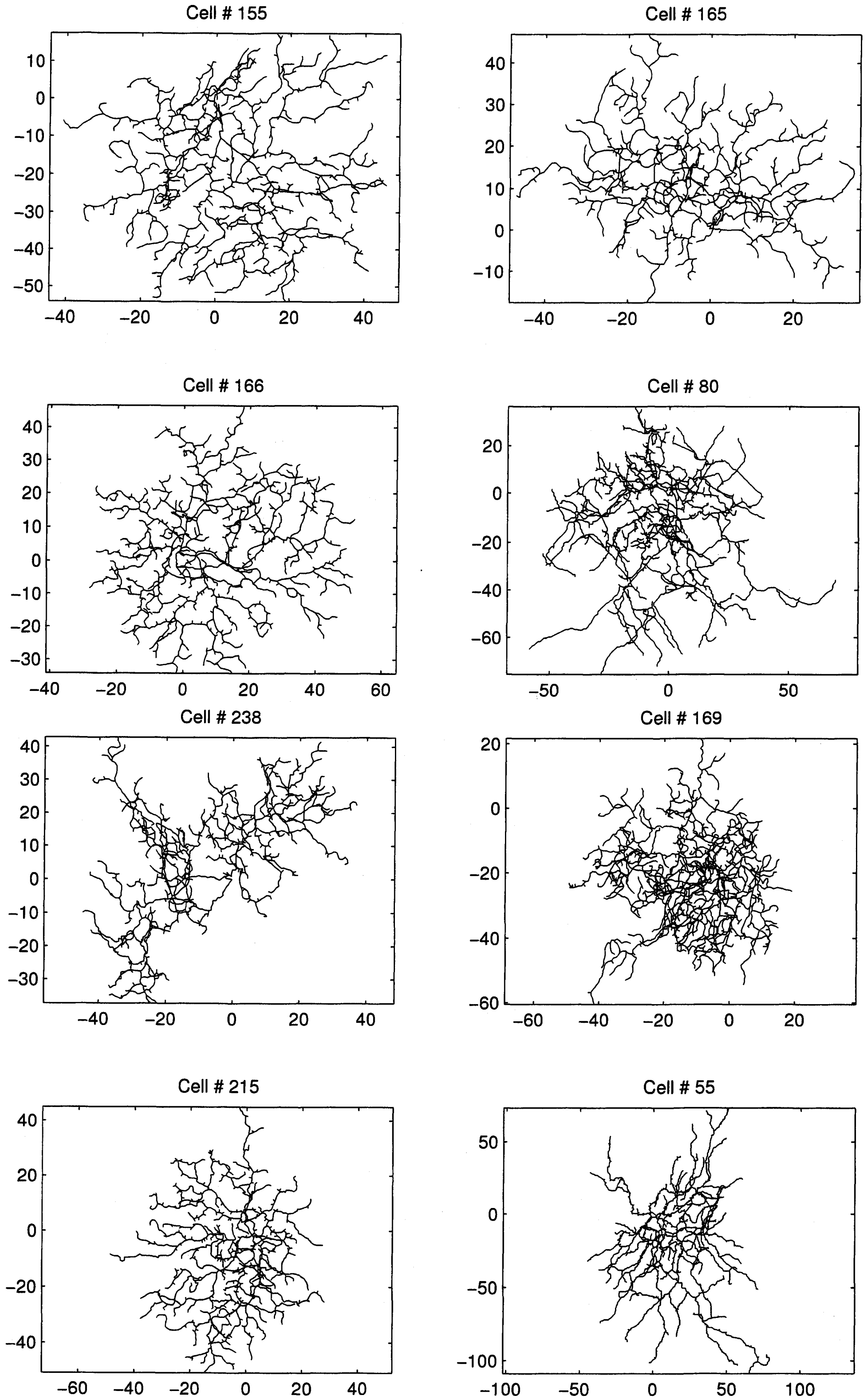
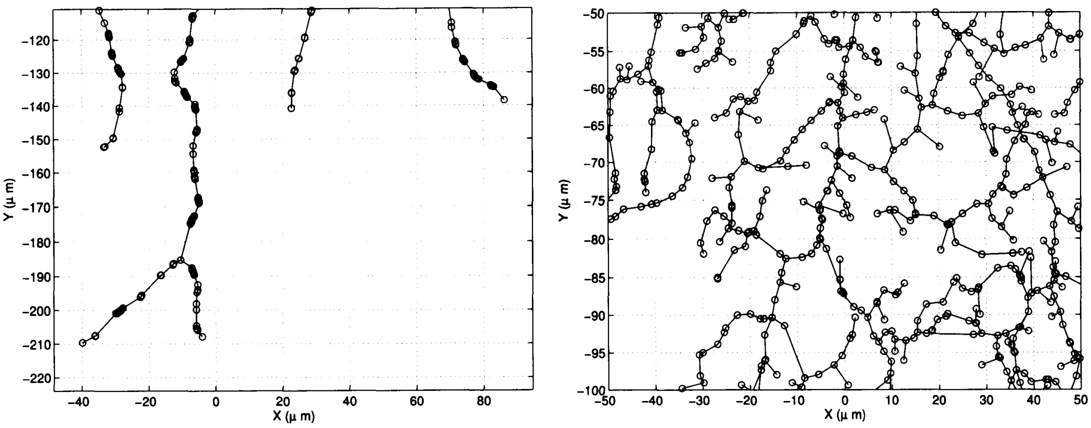


Figure 6: Examples of dendritic trees with $S\ell(T) \lneqq 1$.



(a) RGC #100; $S\ell(T) \equiv 1$ (b) RGC #155; $S\ell(T) = 0.953 \lneqq 1$

Figure 7: Zoomed-up versions of some dendritic trees.

Conjecture 4.1. *For any tree T of finite volume, we have*

$$0 \leq m_T([4,\infty)) \leq \#\{j \in (1,n) \mid d(v_j) \gneqq 2\}$$

and each eigenfunction corresponding to $\lambda \geq 4$ has its largest component (in the absolute value) on the vertices whose degree are larger than 2.

5 A Class of Trees Having the Eigenvalue 4

As raised in Introduction, we are interested in answering Q3: Is there any tree that possesses the exact eigenvalue 4? To answer this question, we have recently found that the following results of Guo [7] (written in our own notation):

Theorem 5.1 (Guo 2006). *Let T be a tree with n vertices. Then,*

$$\lambda_j(T) \leq \left\lceil \frac{n}{n-j} \right\rceil, \quad j = 0, \ldots, n-1,$$

and the equality holds iff a) $j \neq 0$; b) $n-j$ divides n; and c) T is spanned by $n-j$ vertex disjoint copies of $K_{1,\frac{j}{n-j}}$.

This implies the following

Corollary 5.2. *A tree that has an eigenvalue exactly equal to* 4 *necessarily consists of m copies of $K_{1,3} \equiv S(1,1,1)$ connected via their central vertices as shown in Figure 8 where $m \in \mathbb{N}$.*

Proof. Set $n = 4m$ in Guo's theorem. Then, there is an eigenvalue exactly equal to 4 at $j = 3m$, i.e., $\lambda_{3m} = 4$, and this tree necessarily consists of m copies of $K_{1,3}$ connected via their central vertices, which is guaranteed because of the necessary and sufficient conditions in Guo's theorem. □

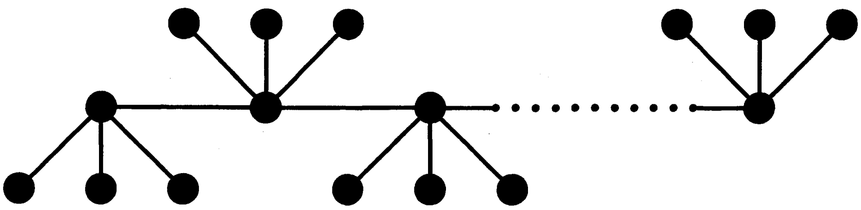


Figure 8: A tree consisting of multiple copies of $K_{1,3}$ connected via their central vertices. This tree has the exact eigenvalue 4 with multiplicity 1.

Figure 9 shows the eigenvalue distribution of a tree consisting of $m = 5$ copies of $K_{1,3}$. Regardless of m, the number of copies of $K_{1,3}$, the eigenfunction corresponding to the eigenvalue 4 has only two values: one constant value at the central vertices, and the other constant value of the opposite sign at the leaves whereas that corresponding to the largest eigenvalue is again concentrated around the central vertex, as shown in Figure 10.

6 Discussion

In this paper, we obtained precise understanding of the phase transition phenomenon of the graph Laplacian eigenvalues and eigenfunctions for starlike trees. For a more complicated class of trees representing dendrites of RGCs, we obtained a conjecture based on the numerical evidence that the number of the eigenvalues larger than 4 is bounded from above by the number of vertices whose degrees is strictly larger than 2. We also identified a special class of trees consisting of copies of the claw $K_{1,3}$, which is the only class of trees that can have the exact eigenvalue 4.

Our next step toward understanding the phase transition phenomenon for real dendritic trees is to analyze a slightly more complicated class of trees, i.e., trees generated by concatenating several starlike trees. Since we now know the eigenvalue/eigenfunction behavior of starlike trees precisely, we expect that we can also shed light on that class of trees. We plan to proceed such analysis by starting with two concatenated starlike trees.

Another quite interesting question is the following. Can a simple (i.e., no multiple edges and no self-loops) and connected graph—not necessarily a tree—have the exact eigenvalue 4? The answer is clear "Yes." For example, a regular finite lattice graph in $\mathbb{R}^d$, $d > 1$ has repeated eigenvalue 4. More precisely, each eigenvalue and the corresponding eigenfunction of a graph representing the regular finite lattice of size $n \times n \times \cdots \times n = n^d$ can be written as

$$\lambda_{j_1,\ldots,j_d} = 4\sum_{i=1}^{d} \sin^2\left(\frac{j_i\pi}{2n}\right) \tag{13}$$

$$\phi_{j_1,\ldots,j_d}(x_1,\ldots,x_d) = \prod_{i=1}^{d} \cos\left(\frac{j_i\pi(x_i+\frac{1}{2})}{n}\right), \tag{14}$$

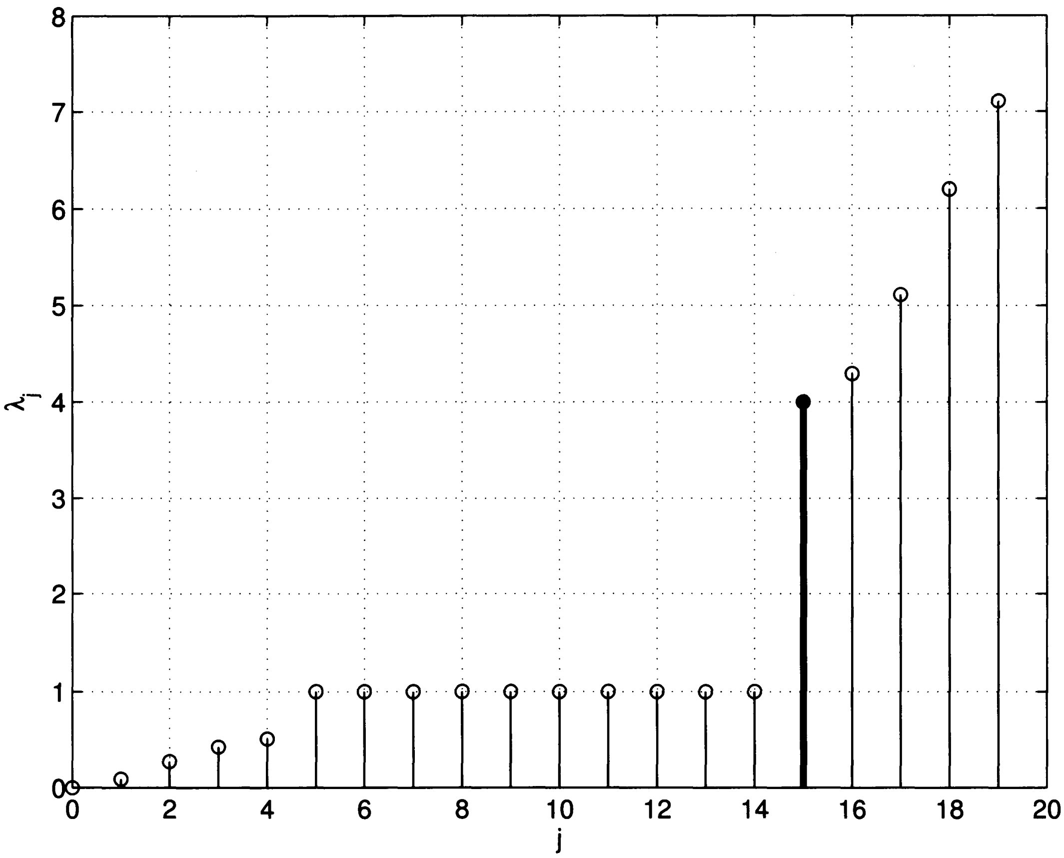
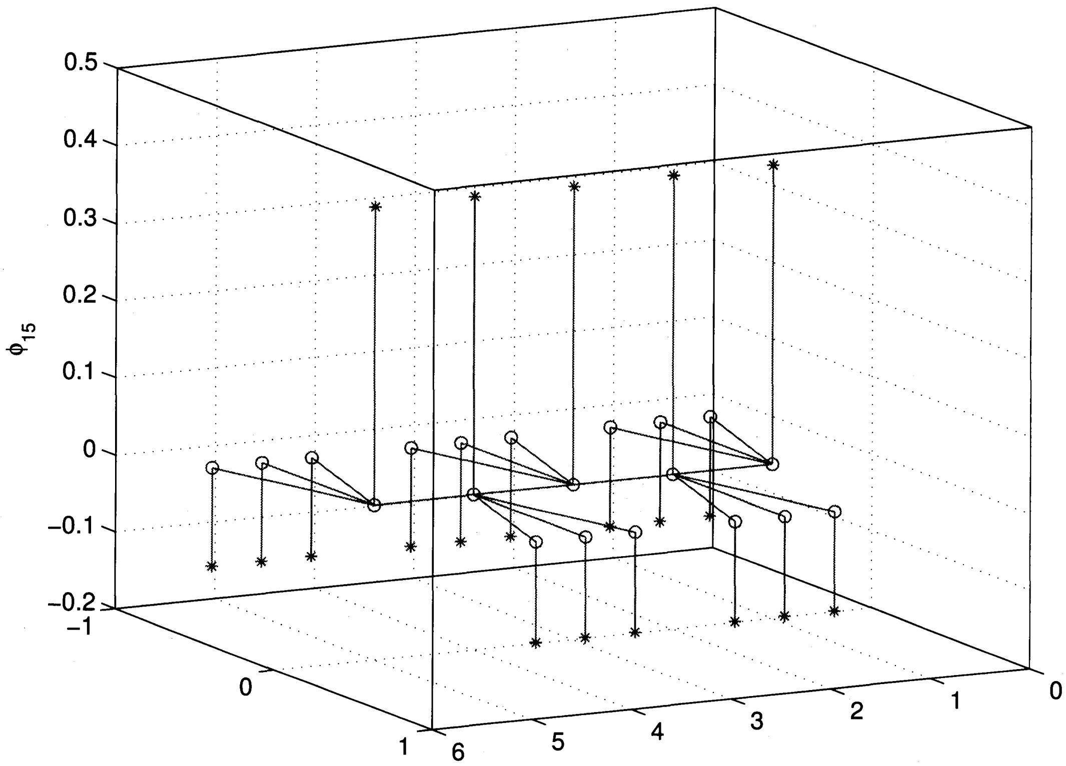
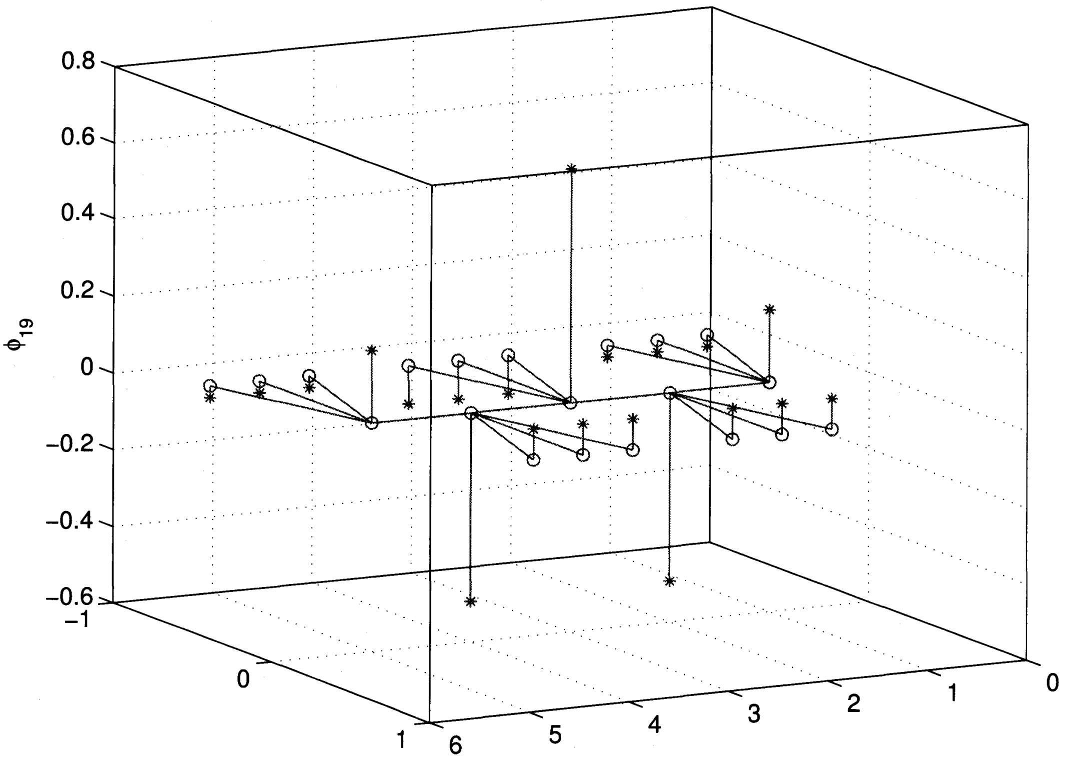


Figure 9: The eigenvalue distribution of a tree consisting of 5 copies of $K_{1,3}$. We note that $S\ell(T) = 1$ for this tree.



(a) ϕ_{15}



(b) ϕ_{19}

Figure 10: (a) The eigenfunction $\boldsymbol{\phi}_{15}$ corresponding to $\lambda_{15} = 4$ of the tree $5K_{1,3}$ in the 3D perspective view. (b) The eigenfunction $\boldsymbol{\phi}_{19}$ corresponding to the maximum eigenvalue $\lambda_{19} = 7.1091$, which shows a bit more concentration around the central vertex.

where $j_i, x_i \in \mathbb{Z}/n\mathbb{Z}$ for each i, as shown by Burden and Hedstrom [2]. Hence, determining $m_G(4)$, i.e., the multiplicity of the eigenvalue 4 of this lattice graph, is equivalent to finding the integer solution $(j_1, \ldots, j_d) \in (\mathbb{Z}/n\mathbb{Z})^d$ to the following equation:

$$\sum_{i=1}^{d} \sin^2\left(\frac{j_i \pi}{2n}\right) = 1. \tag{15}$$

For $d = 2$, it is easy to show that $m_G(4) = n - 1$ by direct examination of (15) with $d = 2$. For $d = 3$, $m_G(4)$ behaves in a much more complicated manner, which is deeply related to number theory. We expect that more complicated situations occur for $d > 3$. We are currently investigating this interesting problem on regular finite lattices with Yuji Nakatsukasa of UC Davis, and we plan to report our findings at a later date. On the other hand, it is clear from (14) that the eigenfunctions corresponding to the eigenvalues greater than or equal to 4 on such lattice graphs cannot be localized or concentrated on those vertices whose degree is larger than 2 unlike the tree case.

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